

# The quantum potential: the breakdown of classical symplectic symmetry and the energy of localisation and dispersion

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The composition of the quantum potential and its role in the breakdown of classical symplectic symmetry in quantum mechanics is investigated. General expressions are derived for the quantum potential in both configuration space and momentum space representations. By comparing the configuration space and momentum space representations of the causal interpretation of quantum mechanics, the quantum potential is shown to break the symplectic symmetry that exists between these two representations in classical mechanics. In addition, it is shown that the quantum potential in configuration space may be expressed as the sum of a momentum dispersion energy and a spatial localisation energy; a complementary expression for the quantum potential being found in the momentum representation. The composition and role of the quantum potential in both representations is analysed for a particle in a linear potential and for two eigenstates of the quantum harmonic oscillator.

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## I. INTRODUCTION

Comparison of classical and quantum dynamics is not only of interest at a fundamental level but is also of particular conceptual and computational value in applications where both classical and quantum phenomena play equally important roles (eg. statistical mechanics, quantum chemistry, molecular dynamics etc). However, such comparison can be hindered by the clear formal differences between classical mechanics and the standard ‘operator’ formalism of quantum mechanics.

A common basis for comparing quantum mechanics and classical mechanics was provided by the introduction of the Wigner distribution function on phase space [1]. It brought to quantum mechanics not only the advantages of C-number only equations but also the appeal of classical concepts that accompany a phase space description. Thus, for example, has the framework of quantum hydrodynamics (QHD) emerged from zeroth, first and second momentum moments of the Wigner distribution and been applied to semi-conductor device modelling [2,3]. In such approaches, separable quantum internal energy terms appear alongside classical thermal pressure and scattering terms. The explicit appearance of an internal energy (or stress) is a result of the projection from the phase space representation to the configuration space representation. This point was made for pure states in quantum me-

chanics by Takabayasi [4] and, more recently, has been demonstrated by Muga et al. [5] for classical mechanics and for pure and mixed states in quantum mechanics.

As noted in [5] and exemplified in [2,3], the quantum contribution can be different in different formalisms and/or approximations. Ferry and Zhou [2] draw attention to the lack of consensus as to the form of the correction potential to be included in the QHD equations used for semi-conductor device modelling. They point out that both the Bohm potential and the Wigner potential have appeared both separately and together in various formulations of QHD. (See references in [2]). Indeed, in [2], Ferry and Zhou find a correction term (hereafter referred to as the Ferry-Zhou potential) which is the difference between the Bohm potential and the Wigner potential as defined in [2]. Implicit in this finding is the observation that the Bohm (quantum) potential is expressible as the sum of two other potentials, at least for a pure quantum state. We make the further observation that little if any attention has been given to the appearance of a quantum potential in the momentum space representation.

The last two observations motivate the present investigation of the composition and role of the (Bohm) quantum potential in quantum mechanics at a more fundamental level. However, rather than starting from a phase space formulation of quantum mechanics, we start from the causal interpretation of quantum mechanics on configuration space. This interpretation offers an alternative basis for direct comparison of quantum and classical dynamics through the Hamilton-Jacobi formalism. In the causal interpretation, the quantum potential, in addition to the external potential, guides the trajectory of the ‘quantum particle’ [6]. The functional form and the effects of the quantum potential in this interpretation have been extensively studied for a wide variety of specific cases [7–13] and in [6].

In this paper, we give equal attention to the expression of the causal interpretation and the appearance of the quantum potential not only in the configuration space representation but also in the momentum space representation. Rather than using a phase space projection to obtain the momentum representation, we use the momentum space representation of the position and momentum operators to obtain the momentum space representation of the quantum Hamilton-Jacobi equations. A comparison of the causal interpretation in its respective configuration space and momentum space representations

provides insight into the classical symplectic symmetry breaking role of the quantum potential.

If the quantum potential reflects the quantum aspects of a system, it should be possible to identify such aspects within the quantum potential. The quantum stress (an energy per unit volume in configuration space) identified by Takabayasi [4], is a measure of momentum dispersion in configuration space and is proportional to the Wigner potential mentioned above. In this paper, we show how in configuration space the balance of the momentum dispersion energy in the Bohm quantum potential is formed by the quantum localisation energy which is the Ferry-Zhou potential also identified above. The latter is proportional to the curvature of the probability density; hence its description as a localisation energy. We also establish the corresponding relationship between the spatial dispersion energy and momentum localisation energy in the momentum space representation. Thus, we find that the balance between localisation and dispersion energies suggests a link between the quantum potential and the Heisenberg uncertainty principle.

The paper is organised as follows. In section II, the appearance of the quantum potential in the standard configuration space representation of the causal interpretation of quantum mechanics is briefly reviewed. In section III, the derivation of the quantum potential is generalised in configuration and momentum space and its emergence from the actions of the respective kinetic and potential energy operators is demonstrated. In section IV, the symplectic structure of the causal interpretation is investigated by expressing its equations in Hamiltonian form. The classical symplectic symmetry breaking property of the quantum potential is demonstrated. In section V, the quantum potential is expressed as the sum of dispersion and localisation energies and a connection with the Heisenberg uncertainty principle is suggested. In section VI, we examine the role and composition of the quantum potential for a particle in a linear potential and for the ground state and second excited state of the harmonic oscillator. We conclude in section VII.

## II. QUANTUM POTENTIAL IN THE CAUSAL INTERPRETATION

The quantum potential emerges from Bohm's Causal Interpretation [14] of quantum mechanics on configuration space, when the substitution  $\psi = Re^{iS/\hbar}$  is made in the Schrödinger equation:

$$i\hbar \frac{\partial \psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi \quad (1)$$

and the real and imaginary parts are separated yielding the equations:

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} + V = 0 \quad (2)$$

and

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \frac{\mathbf{p}}{m} \right) = 0 \quad (3)$$

where  $\rho = |\psi|^2$  and the particle is assumed to have a definite, but unknown, position with a momentum given by

$$\mathbf{p} = \nabla S. \quad (4)$$

The quantum Hamilton-Jacobi equation (2) contains the extra 'quantum potential' term,  $Q = -\frac{\hbar^2}{2m} \frac{\nabla^2 R}{R}$ , which is dependent upon the magnitude of the wavefunction but not upon its phase. Newton's second law is modified by the 'quantum force' term and becomes

$$\mathbf{F} = -\nabla(Q + V). \quad (5)$$

The kinematic relation

$$\mathbf{v} = \frac{\mathbf{j}}{\rho} = \frac{\mathbf{p}}{m}, \quad (6)$$

derived from the identification of the current density  $\mathbf{j}$  in equation (3), allows trajectories to be determined from the integral curves of (4). Since  $S$  is determined by (1), both the trajectory of an individual particle and the evolution of its dynamical variables are determined by the time development of  $\psi$ . Thus, in Bohm's approach, dynamical behaviour may be expressed through, but not derived from, the familiar apparatus of classical mechanics. The conservation equation (3) ensures that if the density of an ensemble of such trajectories is, at any time, proportional to  $\rho$ , then it was and will be so for all time. It should be emphasised that the Bohm formulation of quantum mechanics is an exact expression of the Schrödinger equation and not a WKB approximation as is sometimes suggested.

The motion of a system may be obtained either by integrating (6), or in principle, by integrating the modified Newton's equation (5) with the initial condition satisfying equation (4). However, unlike the external potential, the quantum potential is not a pre-assigned function of the system co-ordinates and can only be derived from the the wavefunction. It is therefore essentially quantum in nature.

## III. GENERALISED DERIVATION OF THE QUANTUM POTENTIAL

We generalise the above derivation of the quantum potential by first writing the Schrödinger equation in the form:

$$i\hbar \frac{\partial \psi}{\partial t} = (T(\hat{p}) + V(\hat{x})) \psi \quad (7)$$

where  $T(\hat{p})$  and  $V(\hat{x})$  are kinetic and potential energy functions of the momentum and position operators  $\hat{p}$  and  $\hat{x}$  respectively. The substitution  $\psi = Re^{iS/\hbar}$  is made recognising that  $R$  and  $S$  are functions of  $x$  (in the configuration space representation) or of  $p$  (in the momentum space representation).

Applying this ansatz in configuration space, with  $\hat{x} = x$  and  $\hat{p} = -i\hbar\nabla_x$ , the real and imaginary parts of the Schrödinger equation become:

$$\frac{\partial S}{\partial t} + \Re\left(\frac{T\psi}{\psi}\right) + V(x) = 0 \quad (8)$$

and

$$\frac{\partial \rho}{\partial t} - \frac{2\rho}{\hbar}\Im\left(\frac{T\psi}{\psi}\right) = 0. \quad (9)$$

Correspondingly, in momentum space, with  $\hat{x} = i\hbar\nabla_p$  and  $\hat{p} = p$ , the real and imaginary parts of the Schrödinger equation are:

$$\frac{\partial S}{\partial t} + T(p) + \Re\left(\frac{V\psi}{\psi}\right) = 0 \quad (10)$$

and

$$\frac{\partial \rho}{\partial t} - \frac{2\rho}{\hbar}\Im\left(\frac{V\psi}{\psi}\right) = 0. \quad (11)$$

The symmetry between these two representations of the Schrödinger equation is clear. In the remaining part of this section we show how both classical-like and quantum terms emerge from equations (8) and (10) and how the quantum terms constitute the quantum potential. Attention is first given to the configuration space representation.

Expanding exponentials, we write the ‘kinetic’ term in (8) as:

$$\Re\left(\frac{\psi^* T\psi}{\rho}\right) = \Re\left(\frac{R(1 - \frac{iS}{\hbar} - \dots)T(\hat{p})R(1 + \frac{iS}{\hbar} - \dots)}{\rho}\right) \quad (12)$$

If  $T(\hat{p})$  is a general but regular function of  $\hat{p}$ , it may be expanded as a power series in  $\hat{p} = -i\hbar\nabla_x$ . The ‘kinetic’ term may then be separated into the sum of two parts:

$$\Re\left(\frac{T\psi}{\psi}\right) = T_h(x) + T_0(x). \quad (13)$$

(See Appendix.)  $T_h(x)$  is an expansion in even positive powers of  $\hbar$  and so tends to zero as  $\hbar$  tends to zero. On the other hand,

$$T_0(x) = T(\nabla_x S) \quad (14)$$

is independent of  $\hbar$  and identifies  $p = \nabla_x S$ .

The same line of argument allows the ‘potential’ term of the Hamilton-Jacobi equation (10) to be separated into:

$$\Re\left(\frac{V\psi}{\psi}\right) = V_h(p) + V_0(p) \quad (15)$$

$V_h(p)$  is in general an expansion in even positive powers of  $\hbar$ . On the other hand,

$$V_0(p) = V(-\nabla_p S) \quad (16)$$

is independent of  $\hbar$  and identifies  $x = -\nabla_p S$ .

In the configuration representation, it is the simple quadratic monomial form of the kinetic energy operator:

$$T(\hat{p}) = \hat{p}^2/2m \quad (17)$$

that leads to the simple one term expression:

$$T_h(x) = -\frac{\hbar^2}{2m} \frac{\nabla_x^2 R}{R}, \quad (18)$$

known as the quantum potential, while

$$T_0(x) = \frac{(\nabla_x S)^2}{2m}, \quad (19)$$

has the same form as the classical kinetic energy.

In the momentum representation, the quantum potential does not, in general, have the simple one term form of the usual configuration space representation. (See Appendix). The free particle aside, there are other exceptions to this rule. For the linear potential  $V(x) \sim x$ , there is no quantum potential in the momentum representation. For the harmonic oscillator potential  $V(x) = \frac{1}{2}m\omega^2$ , the quantum potential has the simple form:

$$V_h(p) = -\frac{\hbar^2}{2}m\omega^2 \frac{\nabla_p^2 R}{R}, \quad (20)$$

while

$$V_0(p) = \frac{(\nabla_p S)^2}{2}m\omega^2 \quad (21)$$

has the same form as the classical potential energy. These equations have the same form as (18) and (19), being likewise generated by a quadratic monomial form.

Potentials,  $V(x)$ , of higher polynomial order generate a series of energy terms contributing to the total quantum potential in the momentum representation. These include the sum of products of derivatives of  $R$  and  $S$  with respect to  $p$ ; all terms having even powers of  $\hbar^2$ . For example, in the monomial case of  $V(x) = x^4$ , the quantum potential in the momentum representation is:

$$V_h(p) = \frac{\hbar^4}{R} \frac{\partial^4 R}{\partial p^4}$$

$$\begin{aligned}
& -6 \frac{\hbar^2}{R} \left( \frac{\partial^2 R}{\partial p^2} \right) \left( \frac{\partial S}{\partial p} \right)^2 - 12 \frac{\hbar^2}{R} \left( \frac{\partial R}{\partial p} \right) \left( \frac{\partial S}{\partial p} \right) \frac{\partial^2 S}{\partial p^2} \\
& - 3 \hbar^2 \left( \frac{\partial^2 S}{\partial p^2} \right)^2 - 4 \hbar^2 \left( \frac{\partial S}{\partial p} \right) \frac{\partial^3 S}{\partial p^3}
\end{aligned} \quad (22)$$

and the external potential is:

$$V_0(p) = \left( -\frac{\partial S}{\partial p} \right)^4 \quad (23)$$

The composition of the quantum potential in the momentum representation is therefore, in general, much harder to evaluate and interpret than in the configuration space representation.

#### IV. THE SYMPLECTIC STRUCTURE OF THE CAUSAL INTERPRETATION

We build upon the previous section by expressing the dynamic (5) and kinematic (6) relations of the causal interpretation in Hamiltonian form using an effective Hamiltonian.

From equations (8), (13) and (14) of the configuration space representation, the causal trajectory moves under the influence of the effective Hamiltonian

$$H_x = T(p) + T_h(x) + V(x), \quad (24)$$

where the identification  $p = \nabla_x S$  is understood. The kinematic and dynamic equations of motion for the trajectory emerge directly from Hamilton's equations:

$$\dot{x} = \left[ \frac{\partial H_x}{\partial p} \right]_{p=\nabla_x S} = \left[ \frac{\partial T(p)}{\partial p} \right]_{p=\nabla_x S} \quad (25)$$

and

$$\dot{p} = -\frac{\partial H_x}{\partial x} = -\frac{\partial (T_h(x) + V(x))}{\partial x}. \quad (26)$$

Similarly, from equations (10), (15) and (16) of the momentum space representation, the causal trajectory moves under the influence of the effective Hamiltonian

$$H_p = T(p) + V_h(p) + V(x), \quad (27)$$

where the identification  $x = -\nabla_p S$  is understood. Using a Legendre transformation, the Hamiltonian form of the kinematic (25) and dynamic (26) equations of motion in configuration space may be converted to momentum space but applied to the effective Hamiltonian (27). Thus,

$$\dot{p} = -\left[ \frac{\partial H_p}{\partial x} \right]_{x=-\nabla_p S} = -\left[ \frac{\partial V(x)}{\partial x} \right]_{x=-\nabla_p S} \quad (28)$$

and

$$\dot{x} = \frac{\partial H_p}{\partial p} = \frac{\partial (T(p) + V_h(p))}{\partial p}. \quad (29)$$

Comparison between equations (25) and (29) and between equations (28) and (26) shows how the precise symplectic symmetry of classical mechanics is broken by the quantum potential terms in momentum and configuration space respectively. Thus, in general, the trajectory  $x_x(t)$  through configuration space is not the same as the trajectory  $x_p(t)$  in momentum space.  $p_p(t)$  and  $p_x(t)$  are, in general, correspondingly different. These differences seem to reflect the complementary dispersions of position and momentum in quantum mechanics and suggest a connection between the breaking of symplectic symmetry by the quantum potential and the Heisenberg uncertainty principle.

#### V. DISPERSION AND LOCALISATION

Insofar as the quantum potential is a uniquely quantum energy, it is natural to enquire of the source of that energy and to try to identify its composition. A single quantum system has kinetic energy and potential energy. However, unlike single classical systems, it also has intrinsic internal energies respectively associated with spatial localisation and momentum dispersion. These quantum features, whose complementary relationship is expressed through the Heisenberg uncertainty relation, form the mechanism by which a quantum system maintains its non-local (ie non-point like) identity in phase space. In the following, we show how, in the configuration space representation, the quantum potential can be expressed as the sum of localisation and dispersion energies. Attention is then given to the same relationship in the momentum space representation.

##### A. Configuration space

In order to develop the link between the quantum potential and localisation and dispersion energies, we first write the quantum potential in configuration space as the sum of two terms:

$$T_h(x) = \frac{-\hbar^2}{2mR} \nabla_x^2 R = M_d(x) + \Sigma_l(x) \quad (30)$$

where

$$M_d(x) = \frac{-\hbar^2}{8m} (\nabla_x^2 \ln \rho) \quad (31)$$

and

$$\Sigma_l(x) = \frac{-\hbar^2}{8m} \left( \frac{\nabla_x^2 \rho}{\rho} \right). \quad (32)$$

The meaning of the suffices is explained below. As mentioned in section I, Ferry and Zhou [2] identify  $M_d(x)$  as the Wigner potential whilst themselves introducing  $\Sigma_l(x)$  (which we call the Ferry-Zhou potential) as the quantum correction potential in their representation of the QHD equations for semi-conductor modelling. Expressing the quantum potential in the form of (30) also allows us to make an important connection with the work of Takabayasi [4] on the quantum mechanics of pure states on phase space.

Takabayasi [4] determines conditions on all distribution moments of the Wigner density  $f(x, p)$  in phase space which guarantee its representing a pure state. These conditions are determined by projections onto configuration space and onto momentum space. Here we present the conditions on the second moments of the distribution  $f(x, p)$  with respect to momentum which apply for the projection onto a one-dimensional configuration space. (The generalisation to all space dimensions is given in [4]). The probability density and the first and second moments of the Wigner density are given by:

$$\rho(x) = \int f(x, p) dp, \quad (33)$$

$$P^{(1)}(x) = \int p f(x, p) dp, \quad (34)$$

and

$$P^{(2)}(x) = \int p^2 f(x, p) dp \quad (35)$$

Defining the mean moments as  $\overline{p(x)} = P^{(1)}(x)/\rho$  and  $\overline{p(x)^2} = P^{(2)}(x)/\rho$ , the lowest order condition on the moments is the dispersion relation:

$$\overline{p(x)^2} - \overline{p(x)}^2 = \frac{-\hbar^2}{4} \nabla_x^2 \ln \rho. \quad (36)$$

Thus,  $M_d(x)$  in (31) is identified as the momentum dispersion energy. Since the Wigner density can be negative for quantum systems, the momentum dispersion can also be negative. In classical ensembles, the momentum dispersion is never negative because the Liouville density in phase space is never negative.

$\Sigma_l(x)$ , in (32), is a measure of the local curvature of the probability density  $\rho$  and we call it the localisation energy for the following reason: It contributes positively to the quantum potential in regions of negative curvature (eg near maxima) and contributes negatively in regions of positive curvature (eg near minima) which correspond to high spatial dispersion. The latter is in contrast to the positive contribution to the quantum potential caused by a high momentum dispersion. The quantum potential in configuration space is therefore the balance between the energies of spatial and momentum dispersion in quantum systems. This balance suggests a link between the

quantum potential and Heisenberg's position-momentum uncertainty principle.

It is important to realise that the above process of projection from phase space onto configuration space can be applied to a classical ensemble of particles each subject to the corresponding classical Hamiltonian. Muga et al. [5] show how this leads to an internal potential in configuration space which appears, in addition to the external potential, in the classical Hamilton-Jacobi equation. As in the quantum case, the internal potential will not vanish unless the momentum dispersion energy vanishes. However, we note here that the quantum (internal) potential is distinguished (at least for a pure state) by being a function of the probability density in  $x$ . In particular, the momentum dispersion energy is dependent upon the density distribution in  $x$ ; a feature certainly absent from the corresponding classical ensemble of non-interacting particles. This inter-dependence of the momentum and configuration space distributions clarifies the link between the quantum potential and the Heisenberg uncertainty principle.

In the causal interpretation of quantum mechanics, the quantum system is represented by an ensemble of particle trajectories (a classical notion) whose density in configuration space is at all times proportional  $\rho(x, t)$ . Each trajectory is not only subject to the external potential,  $V(x)$ , but also to the 'internal' quantum potential,  $T_h(x)$ , which, being composed of the internal energies  $M_d(x)$  and  $\Sigma_l(x)$ , reflects the internal structure of the extended quantum system. Such 'internal' energies are absent from classical particles, because they are points having no inner structure. It is only through ensembles of classical particle trajectories that a representation of the quantum system can be obtained.

We can propose an alternative interpretation that avoids reference to classical particles and treats the quantum system as an extended continuum. In such a model, the quantum potential in  $\delta x$  at  $x$  applies to the fraction  $\rho(x)\delta x$  of the quantum system rather than to the whole system represented as a classical particle at  $x$  with the appropriate probability weighting. The internal energy per unit volume at  $x$  is therefore  $\rho(x)T_h(x)$  and may be described as the internal 'quantum stress' or quantum potential density  $\gamma_h(x)$ . By multiplying (30) throughout by  $\rho(x)$  the quantum potential density,  $\gamma_h(x)$ , may be expressed as the sum of momentum dispersion and the spatial localisation energy densities:

$$\gamma_h(x) = \rho(x)T_h(x) = \mu_d(x) + \sigma_l(x) \quad (37)$$

where

$$\mu_d(x) = \frac{-\hbar^2}{8m} (\rho \nabla_x^2 \ln \rho) \quad (38)$$

and

$$\sigma_l(x) = \frac{-\hbar^2}{8m} (\nabla_x^2 \rho). \quad (39)$$

The energy densities,  $\mu_d(x)$  and  $\sigma_l(x)$ , themselves provide information on the internal structure of the quantum system and result from the projection of Wigner phase space representation of the quantum system onto configuration space.

Takabayasi [4] gives particular attention to the ‘quantum stress’  $-2\mu_d(x)$  whose gradient appears as a source of ‘quantum’ momentum flow in the configuration space momentum conservation equation. This source of momentum flow is in addition to that generated by the gradient of the ‘classical stress’ caused by the external potential. The quantum potential itself only appears as an additive correction to the external potential in the equation for the total time derivative of the momentum. The latter expresses the dynamics of a point moving with the configuration space momentum flow at a velocity of  $\overline{p(x)}/m$  and has precisely the form of equation (5). Here we see that in order to represent quantum dynamics, such a point is subject to forces arising from momentum dispersion and spatial localisation in addition to the external force.

It is easily shown, from (31) and (32), that

$$M_d(x) \geq \Sigma_l(x), \quad (40)$$

and thus

$$\mu_d(x) \geq \sigma_l(x). \quad (41)$$

The equality applies at maxima of the density  $\rho(x)$ , where both energy (density) components contribute equally to the quantum potential (density). This point is illustrated in the examples in section VI.

## B. Momentum space

In the momentum representation, the quantum harmonic oscillator is alone in having a quantum potential in the form:

$$V_h(p) = \frac{-\hbar^2}{2R} m\omega^2 \nabla_p^2 R = \Sigma_d(p) + M_l(p) \quad (42)$$

where

$$\Sigma_d(p) = \frac{-\hbar^2}{8} m\omega^2 (\nabla_p^2 \ln \rho) \quad (43)$$

and

$$M_l(x) = \frac{-\hbar^2}{8} m\omega^2 \left( \frac{\nabla_p^2 \rho}{\rho} \right). \quad (44)$$

We invoke the momentum space position dispersion relation derived for a pure state by Takabayasi [4], by projecting from phase onto momentum space in a manner similar to that described above for configuration space:

$$\overline{x(p)^2} - \overline{x(p)}^2 = \frac{-\hbar^2}{4} \nabla_p^2 \ln \rho. \quad (45)$$

Thus,  $\Sigma_d(p)$ , in (43), is identified as the spatial dispersion energy which can be positive or negative.  $M_l(p)$ , in (44), is the momentum localisation energy term and is proportional to the local curvature of the probability density in momentum space. Therefore, in the momentum representation of the quantum harmonic oscillator, the quantum potential receives positive contributions from the spatial dispersion energy and from the momentum localisation energy. The latter observation complements the similar one made for the configuration space representation, in which the roles of position and momentum are interchanged. Thus, in the momentum representation of the quantum harmonic oscillator also, is the balance of spatial and momentum dispersion suggestive of the Heisenberg uncertainty principle.

As in the configuration space representation, a distinction may be drawn between the trajectory and continuum interpretations of the quantum system in the momentum representation of the quantum harmonic oscillator. Similarly, in the latter interpretation, the quantum potential density,  $v_h(p)$ , can be expressed as the sum of spatial dispersion and momentum localisation energy densities:

$$v_h(p) = \rho(p) V_h(p) = \sigma_d(p) + \mu_l(p) \quad (46)$$

where

$$\sigma_d(p) = \frac{-\hbar^2}{8} m\omega^2 (\rho \nabla_p^2 \ln \rho) \quad (47)$$

and

$$\mu_l(p) = \frac{-\hbar^2}{8} m\omega^2 (\nabla_p^2 \rho). \quad (48)$$

In the case of potentials,  $V(x)$ , of higher polynomial order than two, as shown in (22), the momentum representation yields a multi-termed sum for the quantum potential. Thus decomposition of the quantum potential (density) into the dispersion and localisation energy (densities), as described above, is not possible in general. Therefore, whilst, in correspondence to (40) and (41), the inequalities:

$$\Sigma_d(p) \geq M_l(p) \quad (49)$$

and

$$\sigma_d(p) \geq \mu_l(p) \quad (50)$$

always hold in the momentum representation, in general, the dispersion and localisation energy (densities) do not sum to give the quantum potential energy (density).

## VI. EXAMPLES

To illustrate the discussion of the previous sections, we investigate the symplectic symmetry breaking role and the dispersion and localisation energy components of the quantum potential for two simple systems: a quantum particle in a linear potential and the quantum harmonic oscillator.

### A. The linear potential

#### 1. Configuration space

In the configuration space representation, the stationary one dimensional Schrödinger equation for a particle of mass  $m = 1$  in the potential  $V(x) = x/2$  is:

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{x}{2}\psi = E\psi \quad (51)$$

in units where  $\hbar = 1$ . (For an analysis of this system in quantum phase space see [16]). The physically acceptable solution to this equation is given (up to a multiplicative constant) by the Airy function [15]:

$$\psi(x) = Ai(x - 2E). \quad (52)$$

$x = 2E$  is the turning point of a classical particle trajectory of energy  $E$  initially travelling from  $x = -\infty$  and being reflected by the linear potential at  $x = 2E$  to return to  $x = -\infty$ . Since the potential is unbounded,  $E$  may take on a continuum of values. Without loss of generality, we consider the case  $E = 0$  in which the classical trajectory would be reflected at the origin  $x = 0$ . The density of the wavefunction and the composition of the quantum potential for this system are shown in Fig. 1. At the peaks of the density, the momentum dispersion energy,  $M_d(x)$ , and the spatial localisation energy,  $\Sigma_l(x)$ , (given respectively by (31) and (31)) contribute equally to the quantum potential but become infinite in magnitude at the minima of the density. The quantum potential in the configuration space representation is thus manifested as the sum the energies of momentum dispersion and spatial localisation. As shown in Fig. 2, the quantum potential density and its component energy densities remain finite, with the momentum dispersion energy density showing far less structure than the spatial localisation energy. The kinematic and dynamic equations of motion for the configuration space trajectory are (see equations (25) and (26))

$$\dot{x} = 0 \quad (53)$$

since  $p = \nabla_x S = 0$  for the real wavefunction and

$$\dot{p} = 0 \quad (54)$$

since for stationary systems the quantum potential and external potential sum to the (constant) total energy  $E$ . These equations show that the causal trajectory is a stationary point in configuration space reflecting the exact balance between the (constant) quantum and external forces.

#### 2. Momentum space

In the momentum representation, the stationary one dimensional Schrödinger equation for a particle of mass  $m = 1$  in the potential  $V(x) = x/2$  is:

$$\frac{p^2}{2}\phi + i\frac{1}{2}\frac{\partial\phi}{\partial p} = E\phi \quad (55)$$

in units where  $\hbar = 1$ . The solution to this equation (obtained either directly or by recognising it as the Fourier transform of the Airy function  $Ai(x - 2E)$  in its integral representation [15]) is given (up to a multiplicative constant) by

$$\phi(p) = \exp(2ip(p^2/6 - E)). \quad (56)$$

Maintaining consistency with the configuration space representation, we take  $E = 0$ . As shown in Section III, there is no quantum potential in the momentum space representation of a particle in a linear potential. The kinematic and dynamic equations of motion for the momentum space trajectory are (see equations (29) and (28))

$$\dot{p} = -\frac{1}{2} \quad (57)$$

and

$$\dot{x} = p \quad (58)$$

and are consistent with the causal relation  $x = -\nabla_p S = 2E - p^2$ . The latter equation is also the classical equation of energy conservation for a particle in a linear potential which, in the absence of the quantum potential, has been retrieved from the momentum representation of the causal interpretation of quantum mechanics.

#### 3. Discussion

In this example, the decomposition of the quantum potential (density) into the momentum dispersion energy (density) and spatial localisation (density) is apparent in the configuration space representation but absent in the momentum space representation. In the latter, the constancy of the magnitude of the wavefunction means that both the spatial dispersion and momentum localisation

energies are zero, though, strictly, they cannot be related to the quantum potential in this example.

The example also illustrates how the quantum potential breaks the symplectic symmetry of classical mechanics. In the configuration space representation, the quantum potential acts to cancel the effects of the external potential thus making the trajectory stationary. In the momentum representation, the absence of the quantum potential means that the external potential alone acts upon a causal trajectory, making it identical to the classical trajectory. Furthermore, the absence of the quantum potential and its components makes it impossible, in this case, to adopt an energy density description of the quantum system in the momentum representation.

## B. The quantum harmonic oscillator

### 1. Configuration space

In the configuration space representation, the stationary one dimensional Schrödinger equation for a particle of mass  $m = 1$  in the potential  $V(x) = x^2/2$  is:

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \frac{x^2}{2}\psi = E\psi \quad (59)$$

in units where  $\hbar = 1$ . (For an analysis of this system in quantum phase space see [17]). The eigenfunction corresponding to the  $n^{th}$  eigenvalue,  $E_n = (n + \frac{1}{2})$ , of this equation is well known as:

$$\psi_n(x) = H_n(x)\exp\left(-\frac{x^2}{2}\right) \quad (60)$$

for  $n = 0, 1, 2, \dots$  where  $H_n(x)$  is the  $n^{th}$  Hermite polynomial in  $x$ . Fig. 3 and Fig. 4 respectively show the composition of the quantum potential,  $T_h(x)$ , for the ground state  $\psi_0(x)$  and for the second excited state,  $\psi_2(x)$ . In the ground state (Fig. 3), the momentum dispersion energy,  $M_d(x)$ , is constant, showing that the ‘quantum force’ on causal trajectories arises solely from the variation in the spatial localisation energy,  $\Sigma_l(x)$ . In the case of the second excited state (Fig. 4), variations in both the momentum dispersion and spatial localisation energies contribute to the ‘quantum force’. Fig. 5 and Fig. 6 show the finite components of the quantum potential density for the same two states of the quantum harmonic oscillator. Figs. 3 to 6 clearly illustrate the inequalities (40) and (41). As for the linear potential example, Fig. 6 shows that whilst  $\sigma_l(x)$  is oscillatory,  $\mu_d(x)$  is only very weakly so within the ‘classical domain’ of the quantum system in which the quantum potential (density) is non-negative. Outside this domain, the phenomenon of quantum tunnelling is manifest. The profile of  $\mu_d(x)$ , brings to mind Takabayasi’s observation [4] that ‘...the pressure

in the configuration space ensemble results from the momentum dispersion of the underlying phase space ensemble just in the same manner as the pressure of ideal gas results from the thermal motion of molecules’. However, as far as such analogies can be helpful, in our work here we see that this ‘thermal’ pressure is not alone in contributing to the nett internal pressure (potential energy density) of a quantum system.

The kinematic and dynamic equations of motion for the configuration space trajectory are (see equations (25) and (26))

$$\dot{x} = 0 \quad (61)$$

since  $p = \nabla_x S = 0$  for the real wavefunction and

$$\dot{p} = 0 \quad (62)$$

since for stationary systems the quantum potential and external potential sum to the (constant) total energy  $E$ . As in the case of the linear potential, these equations again show that the causal trajectory is a stationary point in configuration space reflecting the exact balance between the (constant) quantum and external forces.

### 2. Momentum space

In the momentum representation, the Schrödinger equation corresponding to equation (59) is:

$$\frac{p^2}{2}\phi - \frac{1}{2}\frac{\partial^2\phi}{\partial p^2} = E\phi \quad (63)$$

The  $n^{th}$  eigenvalue,  $E_n = (n + \frac{1}{2})$ , has the eigenfunction:

$$\phi_n(p) = H_n(p)\exp\left(-\frac{p^2}{2}\right) \quad (64)$$

for  $n = 0, 1, 2, \dots$  where  $H_n(p)$  is the  $n^{th}$  Hermite polynomial in  $p$ . The form and composition of the quantum potential (density) in the momentum representation (see equations (37) and (46)) can be obtained directly from its form and composition in configuration space by making the symbolic transformations  $x \rightarrow p$ ,

$$M_d(x) \rightarrow \Sigma_d(p), \quad \Sigma_l(x) \rightarrow M_l(p) \quad (65)$$

and

$$\mu_d(x) \rightarrow \sigma_d(p), \quad \sigma_l(x) \rightarrow \mu_l(p). \quad (66)$$

With these substitutions, Figs. 3 to 6 give the form and composition of the quantum potential (density) of the quantum harmonic oscillator in the momentum representation. Observations complementary to those made for the configuration space representation can then be made;



though the parallel analogy of the spatial dispersion energy density  $\sigma_d(p)$  with the pressure of an ideal gas in inverse space is of little value.

The kinematic and dynamic equations of motion for the momentum space trajectories are (see equations (29) and (28))

$$\dot{x} = 0 \quad (67)$$

since  $p = \nabla_x S = 0$  for the real wavefunction and

$$\dot{p} = 0 \quad (68)$$

since the quantum potential and external potential sum to the (constant) total energy  $E$ . Thus in the momentum space also is each causal trajectory a stationary point reflecting the exact balance between the (constant) quantum and external forces.

### 3. Discussion

Contrary to the linear potential case, the quantum harmonic oscillator does not exhibit the general classical symplectic symmetry breaking features of the quantum potential, as the latter exactly cancels the variation of the external potential in both the configuration and momentum space representations. As a result and despite its symplectic symmetry, the causal trajectories of the quantum harmonic oscillator are not classical in either representation. However, the existence of the quantum potential (density) and its components in both configuration and momentum space does allow adoption of an energy density continuum description of the quantum system in both representations.

## VII. CONCLUSION

In this work, we have reviewed the causal interpretation of quantum mechanics with particular emphasis on the composition and role of the quantum potential. Whilst the interpretation is normally presented in configuration space, we have attempted to give equal emphasis to its formulation in both configuration space and momentum space. In doing so, we have demonstrated how, in general, the quantum potential breaks the symplectic symmetry that exists between these two representations in classical mechanics. This has been achieved by applying Hamilton's equations of dynamics to the effective Hamiltonian of the quantum Hamilton-Jacobi equation.

Assuming only general polynomial forms for the kinetic energy operator,  $T(\hat{p})$ , and the potential energy operator,  $V(\hat{x})$ , the corresponding terms in the quantum Hamilton-Jacobi equation are found, in general, to be expressible as power series in  $\hbar^2$  in the configuration space and momentum space representations respectively.

The non- $\hbar$  dependent parts of the series become the corresponding classical energy forms if the causal identifications  $p = \nabla_x S$  and  $x = -\nabla_p S$  are respectively adopted in the configuration space and momentum space representations. The  $\hbar^2$  dependent parts of the power series constitute the quantum potential in the two representations. This series consists of the sum of terms containing products of derivatives of the magnitude and phase of the wavefunction. Only in the common case of  $T(\hat{p}) \sim \hat{p}^2$  in configuration space and in the restricted case of  $V(\hat{x}) \sim \hat{x}^2$  in momentum space does the quantum potential have its familiar single term form proportional to the second derivative of the magnitude of the wavefunction.

In the above latter two cases, the quantum potential has been shown to be the sum of a localisation energy and a dispersion energy through a connection with the Wigner phase space representation of quantum mechanics. These intrinsic internal energies distinguish the extended character of quantum systems from the point-like character of individual classical systems from which they are absent. Expressing these energies in energy density form it has been shown how the latter description complements the normal causal description of probability weighted particle trajectories. Thus, as in the example of the momentum representation of a quantum system in a linear potential, the absence of the quantum potential may be complemented by the presence of non-trivial (in this case, classical) causal trajectories. Equally, as in the example of the quantum harmonic oscillator, the quantum potential may be accompanied by trivial (stationary) causal trajectories.

In summary, the quantum potential breaks the symplectic symmetry of classical mechanics and in its energy density form complements the trajectory description of the causal interpretation quantum mechanics. The complementary aspects of the localisation and dispersion energy components of the quantum potential and their explicit dependence upon the probability density in either momentum or configuration space, can be interpreted as a manifestation of the Heisenberg uncertainty principle and of the extended nature of quantum systems. Since the quantum potential is the only  $\hbar$  dependent energy in the hamiltonian, it is surely the essentially quantum aspect of the causal interpretation. We have seen in this paper how, far from being a redundant concept in the causal interpretation, analysis of the quantum potential provides insight into the differences between the dynamics of classical and quantum mechanics.

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## APPENDIX:

In this appendix we show how the full series expansions of equations (13) and (15) naturally separate into  $\hbar$ -dependent and  $\hbar$ -independent parts. The approach may also be applied to the imaginary part functions in equations (9) and (11). The analysis is explicitly given for the kinetic energy operator,  $T(\hat{p})$ , but follows through in an obviously similar manner for the potential energy operator,  $V(\hat{x})$ . Thus, in the following, references to  $T(\hat{p})$  should be applied to  $V(\hat{x})$  with the appropriate transformation of the independent variable.

It is assumed that  $T(\hat{p})$  is any real linear function of monomials in the orthogonal components of  $\hat{p}$  which span  $L$ -dimensional momentum space:

$$T(\hat{p}) = \sum_l^L \sum_m^{M_l} a_{lm} \hat{p}_l^m. \quad (\text{A1})$$

Thus, there are no terms containing products of different components of the momentum and  $T(\hat{p})$  is a sum of energies, uniquely associated with each momentum component, which can be separately analysed. From here on we therefore limit the analysis to one momentum component and drop the dimensional index  $l$ .

The left-hand side of equation (13) may be expressed as:

$$\Re \left( \frac{T\psi}{\psi} \right) = \frac{\Re (e^{-iS/\hbar} T(\hat{p}) R e^{iS/\hbar})}{R} \quad (\text{A2})$$

where  $\psi = R e^{iS/\hbar}$ . Making the identification  $\hat{p} = -i\hbar \frac{\partial}{\partial x}$  and expanding each of the exponentials as a power series gives

$$\begin{aligned} \Re \left( \frac{T\psi}{\psi} \right) &= \frac{1}{R} \sum_{j,k=0}^{\infty} \sum_m^M a_m (-1)^{j+m} \Re (i^{j+k+m}) \\ &\times \hbar^{m-k-j} \frac{S^j}{(j!k!)} \frac{\partial^m (R S^k)}{\partial x^m} \end{aligned} \quad (\text{A3})$$

The extraction of the real part of the multiple summation means that  $j + k + m \in Z_e$  where  $Z_e$  is the set of even integers. The expression must not change when we add an arbitrary constant to  $S$ , ie it must be independent of a constant shift in phase of the wavefunction. Thus all powers of  $S$  must sum to zero. This imposes the constraint that only  $j = 0$  terms can contribute to the summation. Equally, those parts of the partial derivative in equation (A3) which have non-zero powers of  $S$  as factors cannot contribute to the summation. This means that  $m$  is a maximum upper bound on  $k$ , ie  $k \leq m$ . However, even with this bound the expanded partial derivative will, in general, have parts with  $S$  as a factor. These latter may be eliminated in practice by temporarily setting  $S = 0$  thus retaining only those parts of  $\partial^m (R S^k) / \partial x^m$  which have, as factors, first and higher order derivatives of  $S$ . In summary,

$$\begin{aligned} \Re \left( \frac{T\psi}{\psi} \right) &= \frac{1}{R} \sum_m^M \sum_{k=0, k+m \in Z_e}^m a_m (-1)^m (-1)^{\frac{k+m}{2}} \\ &\times \hbar^{m-k} \frac{1}{(k!)} \left[ \frac{\partial^m (R S^k)}{\partial x^m} \right]_{S:0}, \end{aligned} \quad (\text{A4})$$

in which the subscript  $S:0$  denotes the process of eliminating terms with  $S$  as a factor. The combinations of  $k$  and  $m$  values that contribute to the above sum are shown graphically in Fig. 7. Equation (A4) contains only even non-negative positive powers of  $\hbar$ . The  $\hbar$ -dependent component of the summation consists of terms with positive powers of  $\hbar$  as factors:

$$\begin{aligned} T_{\hbar}(x) &= \frac{1}{R} \sum_m^M \sum_{k=0, k+m \in Z_e}^{<m} a_m (-1)^m (-1)^{\frac{k+m}{2}} \\ &\times \hbar^{m-k} \frac{1}{(k!)} \left[ \frac{\partial^m (R S^k)}{\partial x^m} \right]_{S:0}, \end{aligned} \quad (\text{A5})$$

and the  $\hbar$ -independent component consists only of terms for which  $k = m$ :

$$T_0(x) = \sum_m^M a_m \left( \frac{\partial S}{\partial x} \right)^m. \quad (\text{A6})$$

Making the identification  $p = \nabla_x S$  in (A6) we recover the one dimensional classical form of the kinetic energy function assumed in equation (A1) above. Thus, is the form of equation (13) established.

The demonstration of the form and content of equation (15) in the momentum representation proceeds exactly as above but using  $\hat{x} = i\hbar \frac{\partial}{\partial p}$  and  $x = -\nabla_p S$  in place of the corresponding configuration representation equations. The resulting momentum space equations for the Hamilton-Jacobi potential term exactly mirror (A4), (A5) and (A6), except for an extra  $(-1)^{-m}$  multiplicative term in the  $m^{th}$  term of each series.

Considering the normal form  $T(\hat{p}) = \hat{p}^2/2m$ , equations (A5) and (A6), and inspection of Fig. 7 show how the kinetic term in the configuration space representation of the Hamilton-Jacobi equation consists of only one  $\hbar$ -independent term and one  $\hbar$ -dependent (quantum potential) term. This is similarly the case for the potential term of the quantum harmonic oscillator in the momentum representation. In general, the quantum potential term, in either representation (but more commonly in the momentum representation) may consist of many different terms with a series of different even non-zero powers of  $\hbar$ .

FIG. 1. Energy versus position (configuration space) plot for a quantum system of total energy  $E = 0$  in the potential  $V(x) = x/2$ . (Units:  $\hbar = m = 1$ ). The solid line (in arbitrary units) shows the variation of the density  $\rho$ . The straight dashed line shows  $0.5 \times$  quantum potential:  $T_h(x)/2$ . The latter is the common tangent line for the curves of spatial localisation energy,  $\Sigma(x)$ , and momentum dispersion energy,  $M(x)$ , near their respective maxima and minima.

FIG. 2. Energy density versus position (configuration space) plot for a quantum system of total energy  $E = 0$  in the potential  $V(x) = x/2$ . (Units:  $\hbar = m = 1$ ). The solid line (in arbitrary units) shows the variation of the density  $\rho$ . The dashed lines respectively show  $0.5 \times$  quantum potential density,  $\gamma_h(x)/2$ , the spatial localisation energy density,  $\sigma_l(x)$ , and momentum dispersion energy density,  $\mu_d(x)$ .

FIG. 3. Energy versus position (configuration space) plot for the ground state ( $n = 0$ ) of the quantum harmonic oscillator of total energy  $E = 0$  in the potential  $V(x) = x^2/2$ . (Units:  $\hbar = m = 1$ ). The solid line (in arbitrary units) shows the variation of the density  $\rho$ . The dashed lines respectively show  $0.5 \times$  quantum potential,  $T_h(x)/2$ , the spatial localisation energy,  $\Sigma_l(x)$ , and momentum dispersion energy,  $M_d(x)$ .

FIG. 4. Energy density versus position (configuration space) plot for the ground state ( $n = 0$ ) of the quantum harmonic oscillator of total energy  $E = 0$  in the potential  $V(x) = x^2/2$ . (Units:  $\hbar = m = 1$ ). The solid line (in arbitrary units) shows the variation of the density  $\rho$ . The dashed lines respectively show  $0.5 \times$  quantum potential density,  $\gamma_h(x)/2$ , the spatial localisation energy density,  $\sigma_l(x)$ , and momentum dispersion energy density,  $\mu_d(x)$ .

FIG. 5. Energy versus position (configuration space) plot for the second excited state ( $n = 2$ ) of the quantum harmonic oscillator of total energy  $E = 5/2$  in the potential  $V(x) = x^2/2$ . (Units:  $\hbar = m = 1$ ). The solid line (in arbitrary units) shows the variation of the density  $\rho$ . The dashed lines respectively show  $0.5 \times$  quantum potential,  $T_h(x)/2$ , the spatial localisation energy,  $\Sigma_l(x)$ , and momentum dispersion energy,  $M_d(x)$ .

FIG. 6. Energy density versus position (configuration space) plot for the second excited state ( $n = 2$ ) of the quantum harmonic oscillator of total energy  $E = 5/2$  in the potential  $V(x) = x^2/2$ . (Units:  $\hbar = m = 1$ ). The solid line (in arbitrary units) shows the variation of the density  $\rho$ . The dashed lines respectively show  $0.5 \times$  quantum potential density,  $\gamma_h(x)/2$ , the spatial localisation energy density,  $\sigma_l(x)$ , and momentum dispersion energy density,  $\mu_d(x)$ .

FIG. 7. Plot showing the combinations of  $k$  and  $m$  values that contribute to the kinetic and potential energy terms respectively in the configuration and momentum space representations of the quantum Hamilton-Jacobi equation. See equation (A4) in the Appendix. The circles show combinations that can contribute to the Hamilton-Jacobi kinetic and potential energy terms. Lines of constant even powers of  $\hbar$  are shown dotted.  $k = 0$  is the line of non- $S$  dependent combinations and  $k = m$  is the line of terms contributing to the  $\hbar$ -independent kinetic or potential energy.















